# 3. CHEMICAL AND PHYSICAL INFORMATION

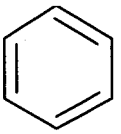
## 3.1 CHEMICAL IDENTITY

Information regarding the chemical identity of benzene is shown in Table 3-l. Although the term benzol is found in older literature for the commercial product, benzene is the name presently approved by the International Union of Pure and Applied Chemistry (IUPAC), the Chemical Manufacturers Association (CMA), and the American Society for Testing and Materials (ASTM) for the pure product (HSDB 1996).

## 3.2 PHYSICAL AND CHEMICAL PROPERTIES

Information regarding the physical and chemical properties of benzene is shown in Table 3-2. The major impurities found in commercial products are toluene, xylene, phenol, thiophene, carbon disulfide, acetylnitrile and pyridine (NIOSH 1974). Commercial refined benzene-535 is free of hydrogen sulfide and sulfur dioxide, but contains a maximum of 1 ppm thiophene and a maximum of 0.15% nonaromatics. Refined nitration-grade benzene is free of hydrogen sulfide and sulfur dioxide. Benzene is also commercially available as thiophene-free, 99 mole%, 99.94 mole% and nanograde quality (HSDB 1996).

## Table 3-1. Chemical Identity of Benzene

| Characteristic | Information | Reference |
|---|---|---|
| Chemical name | Benzene | HSDB 1996 |
| Synonym(s) | Annulene, benzeen (Dutch), benzen (Polish), benzol, benzole; benzolo (Italian), coal naphtha, cyclohexatriene, fenzen (Czech), phene, phenyl hydride, pyrobenzol, pyrobenzole | HSDB 1996 |
| Registered trade name(s) | Polystream | IARC 1982 |
| Chemical formula | $C_6H_6$ | Merck 1989 |
| Chemical structure |  | Merck 1989 |
| Identification numbers: | | |
| CAS registry | 71–43–2 | HSDB 1996 |
| NIOSH RTECS | CY–1400000 | HSDB 1996 |
| EPA hazardous waste | NA | |
| OHM/TADS | 7216601 | HSDB 1996 |
| DOT/UN/NA/IMCO shipping | UN1114; IMO3.2 | HSDB 1996 |
| HSDB | 35 | HSDB 1996 |
| NCI | C55276 | HSDB 1996 |

CAS = Chemical Abstracts Service; DOT/UN/NA/IMO = Dept. of Transportation/United Nations/ North America/International Maritime Dangerous Goods Code; EPA = Environmental Protection Agency; HSDB = Hazardous Substances Data Bank; NCI = National Cancer Institute; NIOSH = National Institute for Occupational Safety and Health; OHM/TADS = Oil and Hazardous Materials/Technical Assistance Data System; RTECS = Registry of Toxic Effects of Chemical Substances

## Table 3-2. Physical and Chemical Properties of Benzene

| Property | Information | Reference |
|---|---|---|
| Molecular weight | 78.11 | Merck 1989 |
| Color | Clear, colorless liquid | Merck 1989 |
| Physical state | Rhombic prisms | HSDB 1996 |
| Melting point | 5.5 °C | Merck 1989 |
| Boiling point | 80.1 °C | Merck 1989 |
| Density at 15 °C, g/cm$^3$ | 0.8787 | Merck 1989 |
| Odor | Aromatic | NFPA 1994 |
| Odor threshold: | | HSDB 1996 |
| Water | 2.0 mg/L | HSDB 1996 |
| Air | 4.9 mg/m$^3$ | |
| Taste threshold: | 0.5–4.5 mg/L | HSDB 1996 |
| Solubility: | | |
| Water at 25 °C | w/w: 0.188% | Merck 1989 |
| Organic solvents | Alcohol, chloroform, ether, carbon disulfide, acetone, oils, carbon, tetrachloride, glacial acetic acid | Merck 1989 |
| Partition coefficients: | | |
| Log $K_{ow}$ | 2.13 | HSDB 1996; Karickhoff 1981; Kenaga 1980 |
| Log $K_{oc}$ | 1.8–1.9 | |
| Vapor pressure at 20 °C | 75 mm Hg | NFPA 1994 |
| Henry's law constant at 25 °C | 5.5x10$^{-3}$ atm-m$^3$/mol | Mackay and Leinonen 1975 |
| Autoignition temperature | 498 °C | NFPA 1994 |
| Flashpoint | –11 °C (closed cup) | Merck 1989 |
| NFPA Hazard Classification: | | |
| Health | 2.2 | HSDB 1996 |
| Flammability | 3.3 | |
| Reactivity | 0.0 | |
| Flammability limits in air | 1.2% (lower limit; 7.8% (upper limit) | NFPA 1994 |
| Conversion factors | 1 ppm = 3.24 mg/m$^3$ at 20 °C and 1 atm pressure; 1 mg/m$^3$ = 0.31 ppm | HSDB 1996 |
| Explosive limits | 1.4% (lower limit); 8% (upper limit) | HSDB 1996 |

NFPA = National Fire Protection Association